Pipecolic acid, N-propoxycarbonyl-, undecyl ester

Inchi: InChI=1S/C21H39NO4/c1-3-5-6-7-8-9-10-11-14-18-25-20(23)19-15-12-13-16-22(19)21(2

InchiKey: BHHYUUOQDGZQSE-UHFFFAOYSA-N

Formula: C21H39NO4

SMILES: CCCCCCCCCCCOC(=O)C1CCCCN1C(=O)OCCC

Mol. weight [g/mol]: 369.54

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.89		Crippen Method
logp	5.462		Crippen Method
mcvol	320.750	ml/mol	McGowan Method
rinpol	2571.00		NIST Webbook
rinpol	2571.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U393002&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

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